

Supporting Information

Host-Guest Interactions and Orientation of Dyes in the One-Dimensional Channels of Zeolite L

by

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Zeolite L (ZL) synthesis. Barrel-shaped ZL crystals were synthesized following the procedure reported in ref. [10] with an oxide ratio of 2.83 K₂O : 1.00 Al₂O₃ : 9.83 SiO₂ : 165.6 H₂O. Usually two 40 ml PTFE pressure vessels were used per synthesis run and the two components for the synthesis gel were prepared as follows. An aluminate solution (solution A) was prepared by first dissolving 8.1 g of potassium hydroxide (Fluka, purum p. a. $\geq 85\%$) in 25.4 g of doubly distilled water. Once the KOH was fully dissolved, 3.5 g of aluminum hydroxide (ABCR, dried gel, $\geq 99\%$) were added and the solution refluxed at 120 °C for 16 h. The slightly turbid solution was then cooled down to r. t. and water loss was compensated. The silica solution (solution B) was prepared by adding 30.2 g of doubly distilled water to 12.9 g of Aerosil OX-50 (Degussa). The mixture was dispersed with an Ultra Turrax T18 basic (IKA) for 15 min at 16000 rpm. The dispersion was left standing at r. t. for 1 h before dispersing it again for 8 min at 16000 rpm.

After this second dispersion step, solution A was quickly poured into solution B under vigorous stirring. The resulting viscous white gel was aged for 3 min at r. t. under strong stirring before being evenly split on the two pressure vessels with a filling height corresponding to ca. $\frac{3}{4}$ of the vessels total volume.

Crystallization took place in a rotating oven at 160 °C for 42 h with a rotation speed of 20 rpm. Once the reaction was finished, the vessels were cooled in an ice bath for 1 h before opening them. The milky white suspension was centrifuged for 15 min at 3100 rpm. The white residue was then washed with boiling doubly distilled water until the pH of the supernatant was 7.

Table S1. Numerical values extracted from the aqueous solution spectra shown in Figure 2.

Electronic transitions	Vibronic transition, absorption	Energy [10^3 cm^{-1}]	Difference [10^3 cm^{-1}]	Vibronic transition, fluorescence	Energy [10^3 cm^{-1}]	Difference [10^3 cm^{-1}]
$S_0 - S_1$ (1L_a)	0-0'	22.7		0'-0	22.7	
	0-1'	24.0	1.3	0'-1	21.5	1.2
	0-2'	25.3	1.3	0'-2	20.3	1.2
	0-3'	26.5	1.2	0'-3	19.2	1.1
				0'-4	17.5	1.3
				0'-5	16.3	1.2
$S_0 - S_2$ (1L_b)	0-0''	28.0				
	0-1''	29.3	1.3			

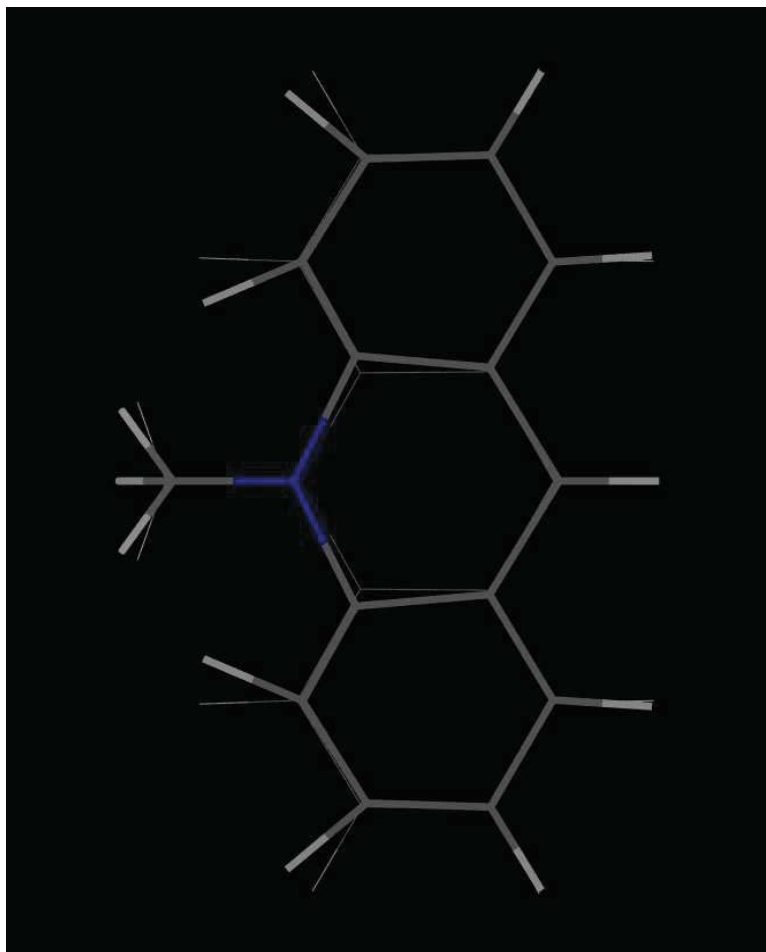


Figure S1. Deformation (thick lines) of the A' mode at 1300 cm^{-1} with respect to the ground state structure (thin lines). Color codes: gray, C atoms; blue N atom; white, H atoms.

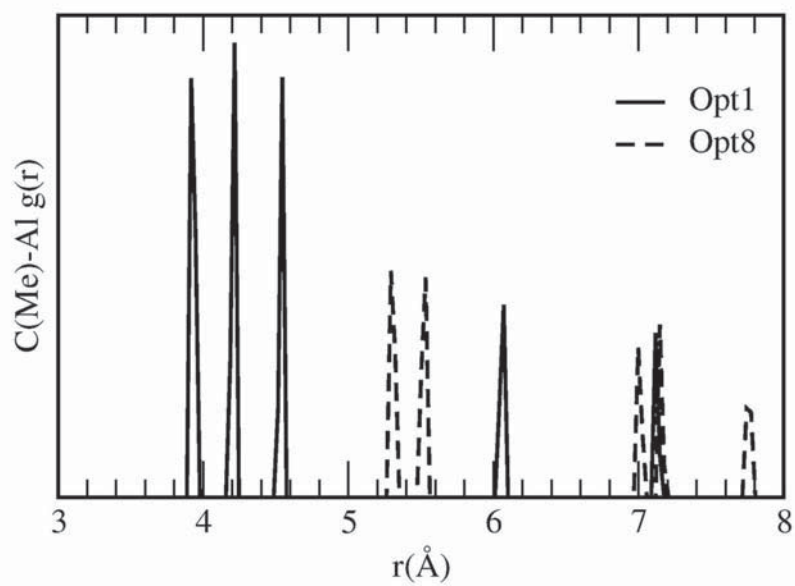


Figure S2. Radial distribution function $g(r)$ involving the C atom of the methyl group of MeAcr^+ and the Al atoms in the zeolite framework, obtained for the optimized dry structures Opt1 (continuous line) and Opt8 (dashed line)

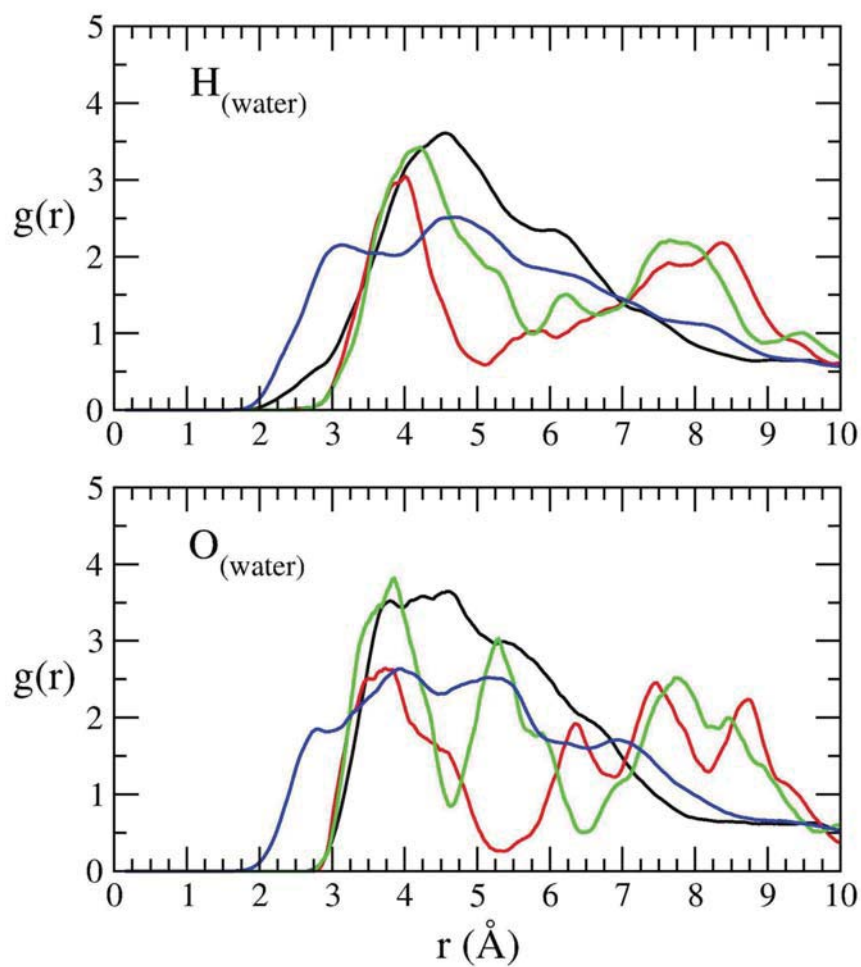


Figure S3. Radial distribution function $g(r)$ from MD1 trajectory. Top panel: $g(r)$ for $H_{(water)}$ with $MeAcr^+$ atoms; bottom panel: $g(r)$ for $O_{(water)}$ with $MeAcr^+$ atoms. Color codes: black, C atoms of the aromatic rings; red, C atom of methyl group; green, N atom, blue, H atoms.

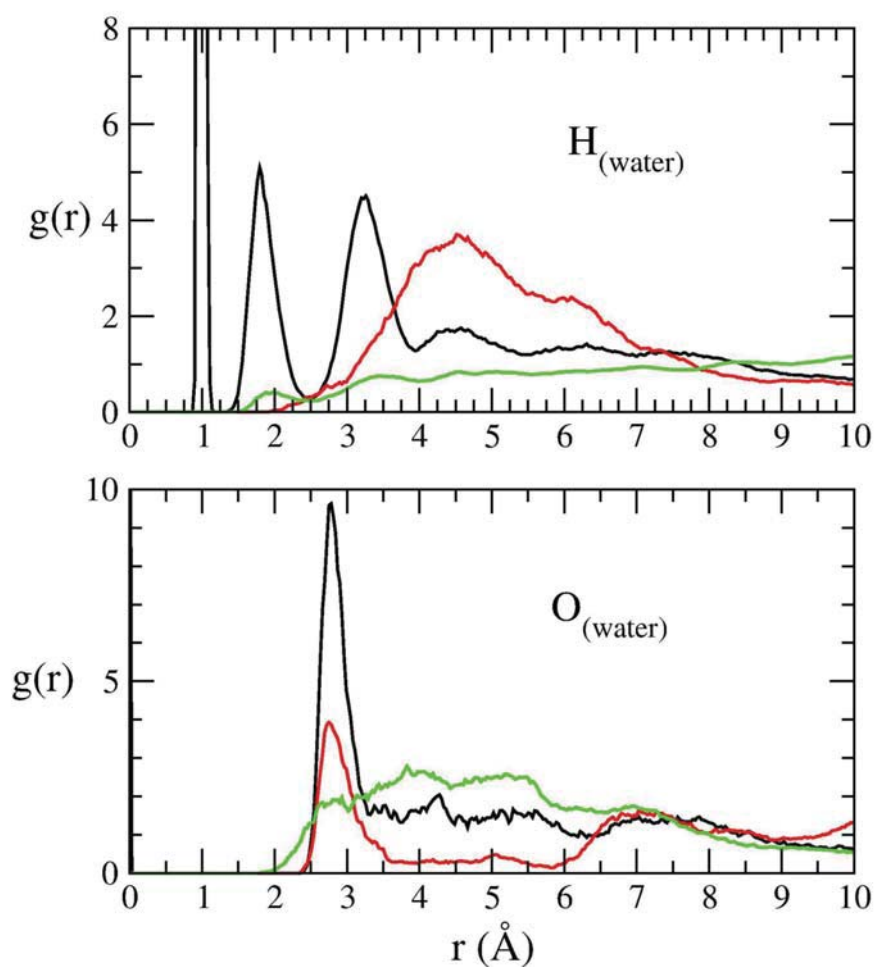


Figure S4. Radial distribution function $g(r)$ from MD1 simulation. Bottom panel: $g(r)$ involving O(water). Top panel: $g(r)$ involving H(water) atoms. Color codes: O(water) in black, K^+ in red, O(zeolite) in green.

Enhanced web object: Movie1. Mpeg movie illustrating the mobility of a $MeAcr^+$ dye molecule inside a dry $MeAcr^+$ -ZL system.